Advanced Materials Research Vols. 93-94 (2010) pp 35-38
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doi:10.4028/www.scientific.net/AMR.93-94.35

Using Polymer Electrolyte Membranes as Media to Culture Fractals: A Simulation Study

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Keywords: Polymer Electrolytes, Culture, Fractals, Simulation.

Abstract. In the authors' laboratory, fern-like fractals have been cultured in polymer electrolyte membranes of polyethylene oxide (PEO) doped with ammonium iodide (NH_4I). The simulation study was then carried out utilizing the Diffusion Limited Aggregation (DLA) based on random motion of aggregating particles modelling technique. The fractal dimension values and the forms of the simulated fractals are comparable to those observed in the PEO polymer membranes. These indicate that the simulation using the DLA model done in this study has resulted outputs that are in abidance with the original fractals cultured in the polymer membranes.

Introduction

In general, polymer electrolytes may be defined as membranes that possesses transport properties comparable with that of common liquid ionic solutions. In the last three decades, the development of polymer electrolytes has drawn the attention of many researchers [1] due to their potential applications not only in batteries but also in devices such as fuel cells, supercapacitors, sensors, electrochromic displays, and solar cells.

Many of fractal growth models are suitable with experimental phenomena such as electrochemical electrodeposition [2], electrochemical polymerization [3] and Diffusion Limited Aggregation growth structures of many metal aggregates in the presence of a magnetic field as external stimuli [4]. The formation of fractals without using any external stimuli has been reported by a few groups of researchers [3, 5-9]. In this work, fern-like fractals have been cultured using polyethylene oxide-ammonium iodide (PEO-NH_4I) electrolytes membranes as the growth media. The growth of these fractals is attributed to the diffusion of ions in the polymer matrix. A computerize based model has been created to simulate the fractal patterns. The model was studied and a computer program to simulate the fractal growth patterns has been developed. In the process of developing the simulation model, studies were carried out on related issues such as the fractal growth patterns and mechanism, and characteristics of the fractals.

Materials and Methods

Materials preparation. The polymer electrolyte membranes used as media to culture fractals were prepared by using the solution casting method. In this preparation, PEO ($M_w = \sim 6 \times 10^5$) and NH_4I were weighed in desired PEO:NH_4I weight ratios and dissolved in 100 ml methanol using digital magnetic stirrers. The mixtures were stirred for hours until homogeneous solutions were obtained. Each solution that had completely dissolved was then cast into petri dishes and left to dry slowly at room temperature in a dark and dry place for several weeks. After drying, fractal patterns were observed and their digital images were taken.

Simulation methods. The fractal patterns obtained in the PEO-NH_4I membranes look similar to fractal-like aggregation usually found in large size isotropic fractal patterns such as Diffusion Limited Aggregates (DLA) in ion conducting polymeric system [6]. In order to simulate the fractal patterns, the simulation of DLA model on a square lattice has been applied. Simulation of the DLA model gives a simple yet effective way to represent fractals obtained in the present work as this simulation technique follows the Brownian motion theory. Fig. 1 depicts a simple representation of a basic DLA model of aggregation of particles.

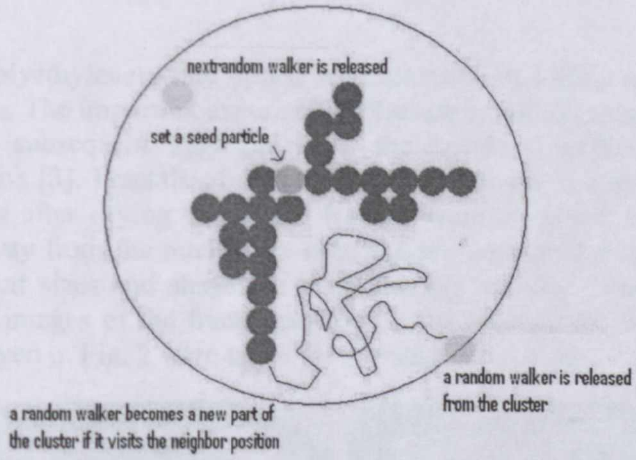


Fig. 1: An off the scale model of aggregation of cluster particles

Determination of fractal dimensions. Fractal dimension is a measure of how complicated a self-similar figure is. The fractal dimension is often fractional. For aggregates, a fractal dimensionality in terms of scaling relationship between two different aggregates' properties X and Y (e.g. mass and length) can be observed such as:

$$Y \propto X d_f \tag{1}$$

where d_f = all purpose fractal dimension as described by Meakin [10].

In fractal geometry, box-counting dimension is a way of determining the fractal dimension of a set S in a Euclidean space R^n. To calculate this dimension for a fractal S, imagine this fractal lying on an evenly-spaced grid, then the number of boxes required to cover the set is counted. The box-counting dimension is calculated by seeing how this number changes as the grid becomes finer.

Suppose that $N(s)$ is the number of boxes of side length s required to cover the set [11], then S has box dimension D if $N(s)$ satisfies the power law

$$N(s) \approx c(1/s)^D \tag{2}$$

asymptotically in the sense that

$$\lim_{s \to 0} N(s)s^D = c \tag{3}$$

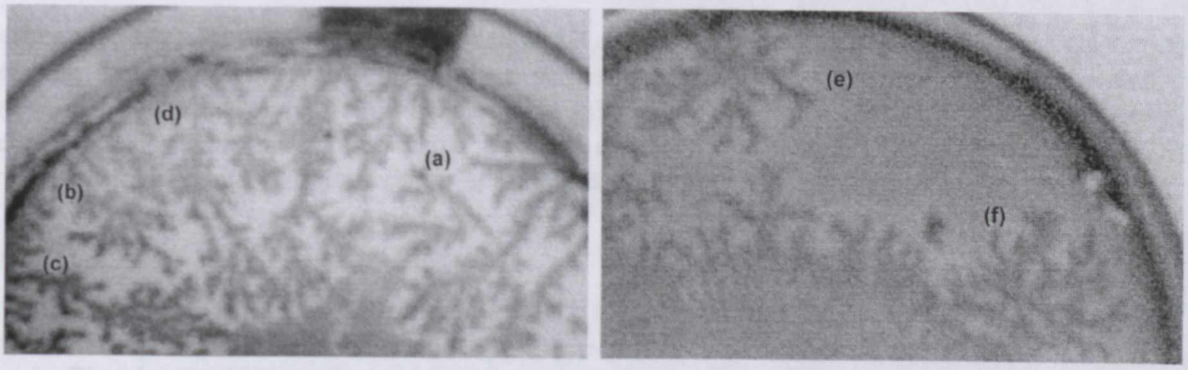
By solving Eq. 2 asymptotically for D, the box-counting dimension is computed as:

$$D = \lim_{s \to 0}\left[-\frac{\log N(s)}{\log s}\right] \tag{4}$$

In this work, the box-counting method was used to determine the fractal dimension. The box counting method has succeeded in giving a systematic measurement for any structure in a 2 dimensional plane and can be adapted for structures in 3 dimensional spaces. It can also be used to conduct both textural and structural analysis of a structure [12]. This method is indeed a very useful method as it is very flexible. Basically, to determine a dimension, a square mesh (grid) of various sizes s was laid over the simulated image (containing the object). The numbers of mesh boxes $N(s)$ that contain the image were counted. The fractal (box) dimension D is given by the slope of the linear portion of a log ($N(s)$) versus log ($1/s$) graph.

Discussion

In the present work, polyethylene oxide doped with ammonium iodide membranes were used as media for fractal growth. The important experimental feature is that no external bias was applied for either the creation or subsequent aggregation of the 'random walkers/ions' as done in the electrodeposition systems [3]. Fractals of different sizes as shown in Fig. 2 were observed in the PEO-NH_4I films weeks after drying time. The fractals were observed to grow from nucleation centers in directions away from the nucleation sites and are separated from each other by definite boundaries. The different sizes and shapes of these fractals are due to the effect of neighboring fractal aggregates. The images of the fractal patterns in the membranes with different polymer to salt weight ratios displayed in Fig. 2 were taken for simulation purposes.



70:30 weight ratio 60:40 weight ratio

Fig. 2: Digital images of the fractal patterns observed in PEO-NH_4I membranes of different polymer:salt weight ratios

Fractal dimension values of the selected fractals in the polymer membranes were determined using a computer software tool, utilizing the box-count method, developed by the authors [13]. The fractal dimensions of the simulated fractals were calculated by a subsection of the programming code which is also based on the box-count method, incorporated in the computer program which runs the simulation. For this simulation work, six fractal aggregates (Fig. 2 (a-f)) were selected. Their simulated patterns are shown in Fig. 3.

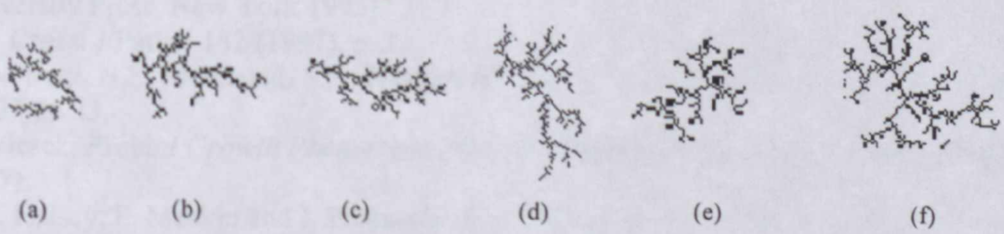


Fig. 3: The simulated fractal patterns.

The simulated fractal patterns shown in Fig. 3 show remarkable resemblance to the original DLA type fractals cultured in the laboratory. The fractal dimension values for all of the simulated and experimentally cultured fractals of various sizes are listed in Table 1. The table shows that the fractal dimension values obtained were found to be ~1.7 which is typical for DLA type fractals as proven by Vicsek [14] and Halsey et al [15]. Furthermore, percentage of differences for both experimentally and simulated patterns are found to be so small with the highest and lowest percentage of difference of 0.199% and 0.065% respectively. The table also shows that the fractal dimension values of the simulated fractals are in good agreement with the fractal dimension values obtained from their respective experimentally obtained ones.

Table 1. Fractal dimension values of the simulated fractal patterns and their respective experimentally cultured fractal patterns.

Fractal dimension of the Experimentally cultured fractals		Fractal dimension of the simulated fractals using DLA model		Percentage of difference (%)
Fig. 2(a)	1.734 ± 0.051	Fig. 3(a)	1.740 ± 0.048	0.199
Fig. 2(b)	1.748 ± 0.045	Fig. 3(b)	1.751 ± 0.044	0.098
Fig. 2(c)	1.759 ± 0.052	Fig. 3(c)	1.763 ± 0.041	0.129
Fig. 2(d)	1.769 ± 0.047	Fig. 3(d)	1.763 ± 0.040	0.192
Fig. 2(e)	1.755 ± 0.039	Fig. 3(e)	1.757 ± 0.042	0.065
Fig. 2(f)	1.786 ± 0.048	Fig. 3(f)	1.789 ± 0.045	0.094

Conclusion

The fractal patterns formed were recognized as DLA type fractals. The success in growing fractals using the PEO based polymer membranes shows that besides applications in electrochemical devices, polymer electrolyte membranes are also suitable for the study of fractals. The results of the studies also show that the model which is based on the Brownian motion theory is pertinent to fractals cultured in the PEO-NH_4I polymer membranes.

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